Metal/Catalyst-Free Sequential C-N Bond Forming Cascades at Room Temperature: Environment-Friendly One-Pot Synthesis of 5-Aminoimidazoles from Aryl Glyoxals, Anilines and Amidines

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Table 1. Optimization of the Reaction Conditions

<table>
<thead>
<tr>
<th>Entry</th>
<th>Stoichiometry</th>
<th>Condition</th>
<th>Yield %</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1a + 2a (1.0 equiv.) in EtOH, stir for 1 h; then 3a-HCl (1.1 equiv.) + TEA (1.5 equiv.)</td>
<td>55 °C, 6 h</td>
<td>56</td>
</tr>
<tr>
<td>2</td>
<td>1a + 2a (1.0 equiv.) in EtOH, stir for 1 h; then 3a-HCl (1.1 equiv.) +K₂CO₃ (1.5 equiv.)</td>
<td>55 °C, 6 h</td>
<td>58</td>
</tr>
<tr>
<td>3</td>
<td>1a + 2a (1.0 equiv.) in EtOH, stir for 2 h; then 3a-free base (1.1 equiv.)</td>
<td>55 °C, 6 h</td>
<td>60</td>
</tr>
<tr>
<td>4</td>
<td>1a (1.0 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>62</td>
</tr>
<tr>
<td>5</td>
<td>1a (1.1 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>73</td>
</tr>
<tr>
<td>6</td>
<td>1a (1.2 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>86</td>
</tr>
<tr>
<td>7</td>
<td>1a (1.3 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>83</td>
</tr>
<tr>
<td>8</td>
<td>1a (1.2 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then 3a (1.8 equiv.)</td>
<td>RT, 16 h</td>
<td>68</td>
</tr>
<tr>
<td>9</td>
<td>1a (1.2 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.2 equiv.)</td>
<td>RT, 16 h</td>
<td>86</td>
</tr>
<tr>
<td>10</td>
<td>1a (1.3 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>55 °C, 16 h</td>
<td>69</td>
</tr>
<tr>
<td>11</td>
<td>1a (1.3 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h 50 °C; then 3a (2.0 equiv.)</td>
<td>55 °C, 16 h</td>
<td>49</td>
</tr>
<tr>
<td>12</td>
<td>1a (1.2 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then AcOH (0.2 equiv.) 3a (2 equiv.)</td>
<td>RT, 16 h</td>
<td>50</td>
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<tr>
<td>13</td>
<td>1a (1.2 equiv.) in MeOH, + 2a (1.0 equiv.) stir for 3 h; then p-TSA (0.2 equiv.) 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>73</td>
</tr>
<tr>
<td>14</td>
<td>1a (1.2 equiv.) in EtOH, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>68</td>
</tr>
<tr>
<td>15</td>
<td>1a (1.2 equiv.) in IPA, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>55</td>
</tr>
<tr>
<td>16</td>
<td>1a (1.2 equiv.) in THF, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>18</td>
</tr>
<tr>
<td>17</td>
<td>1a (1.2 equiv.) in DMF, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>07</td>
</tr>
<tr>
<td>18</td>
<td>1a (1.2 equiv.) in DMSO, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>13</td>
</tr>
<tr>
<td>19</td>
<td>1a (1.2 equiv.) in ACN, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>22</td>
</tr>
<tr>
<td>20</td>
<td>1a (1.2 equiv.) in DCM, + 2a (1.0 equiv.) stir for 3 h; then 3a (2.0 equiv.)</td>
<td>RT, 16 h</td>
<td>20</td>
</tr>
</tbody>
</table>

*a All reactions were performed with 2a (1.0 mmol).*
General procedure one-pot synthesis of highly substituted imidazoles (4a-4aq).

Aniline (1.0 mmol) was added to a stirred solution of glyoxal (1.2 mmol) in MeOH (5 mL) and stirred for 1.5 h at rt. To this mixture, benzaimidine (2.0 mmol) was added and stirred for additional 16 h. The reaction mass was concentrated under reduced pressure and the residue was purified by silica gel column chromatography (EtOAc in n-hexane).

2,4-Diphenyl-N-(p-tolyl)-1H-imidazol-5-amine (4a).

Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4a as white solid (0.28 g, yield 88%), mp 145–147 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.93 (d, $J = 7.6$ Hz, 2H), 7.73 (d, $J = 7.2$ Hz, 2H), 7.44 (t, $J = 7.6$ Hz, 2H), 7.37 (d, $J = 7.2$ Hz, 1H), 7.31 (t, $J = 7.6$ Hz, 2H), 7.19 (t, $J = 7.2$ Hz, 1H), 6.92 (d, $J = 8.0$ Hz, 2H), 6.63 (d, $J = 8.0$ Hz, 2H), 2.18 (s, 3H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 145.89, 145.34, 131.39, 130.51, 129.82, 129.69, 129.49, 128.23, 127.66, 126.96, 126.60, 114.93, 20.55. HRMS (ESI) m/z: [M + H]$^+$ calcd for C$_{22}$H$_{20}$N$_3$ 326.1657; found 326.1648.

N,2,5-Triphenyl-1H-imidazol-5-amine.
Purification by silica gel column chromatography (0 to 13% EtOAc in n-hexane) afforded 4b as light yellow solid (0.22 g, yield 71%), mp 158–160 °C. \(^1\)H NMR (400 MHz, CD\(_3\)OD): \(\delta\) 7.94 (d, \(J = 8.8\) Hz, 2H), 7.74 (d, \(J = 8.4\) Hz, 2H), 7.45 (t, \(J = 8.4\) Hz, 2H), 7.39 (t, \(J = 7.6\) Hz, 1H), 7.32 (t, \(J = 7.6\) Hz, 2H), 7.20 (t, \(J = 7.6\) Hz, 1H), 7.10 (t, \(J = 8.8\) Hz, 2H), 6.72 (d, \(J = 8.0\) Hz, 2H), 6.67 (t, \(J = 8.8\) Hz, 1H); \(^13\)C NMR (100 MHz, CD\(_3\)OD): \(\delta\) 148.35, 145.47, 131.36, 130.03, 129.82, 129.73, 129.51, 127.75, 126.98, 126.62, 119.11, 114.82. HRMS (ESI) \(m/z\): [M + H]\(^+\) calcd for C\(_{21}\)H\(_{18}\)N\(_3\) 312.1501; found 312.1489.

*N-(4-(Tert-butyl)phenyl)-2,4-diphenyl-1H-imidazol-5-amine (4c).*

Purification by silica gel column chromatography (0 to 20% EtOAc in n-hexane) afforded 4c as white solid (0.32 g, yield 86%), mp 208–209 °C. \(^1\)H NMR (400 MHz, CD\(_3\)OD): \(\delta\) 7.94 (d, \(J = 8.0\) Hz, 2H), 7.75 (d, \(J = 7.2\) Hz, 2H), 7.45 (t, \(J = 7.6\) Hz, 2H), 7.38 (d, \(J = 7.2\) Hz, 1H), 7.33 (t, \(J = 7.2\) Hz, 2H), 7.21 (d, \(J = 7.6\) Hz, 1H), 7.16 (d, \(J = 7.6\) Hz, 2H), 6.67 (d, \(J = 8.0\) Hz, 2H); \(^13\)C NMR (100 MHz, CD\(_3\)OD): \(\delta\) 145.88, 145.38, 141.93, 131.47,
129.88, 129.75, 129.56, 127.72, 127.02, 126.83, 126.66, 114.65, 34.74, 32.06. HRMS (ESI) m/z: [M + H]+ calcd for C_{25}H_{26}N_{3} 368.2127; found 368.2118.

N-(4-Methoxyphenyl)-2,5-diphenyl-1H-imidazol-5-amine (4d).

![Chemical Structure of 4d](image)

Purification by silica gel column chromatography (0 to 17% EtOAc in n-hexane) afforded 4d as brown solid (0.24 g, yield 71%), mp 175−177 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.94 (d, $J$ = 8.8 Hz, 2H), 7.74 (d, $J$ = 7.2 Hz, 2H), 7.45 (t, $J$ = 7.2 Hz, 2H), 7.38 (d, $J$ = 7.6 Hz, 1H), 7.32 (t, $J$ = 8.0 Hz, 2H), 7.20 (t, $J$ = 7.6 Hz, 1H), 6.74 (d, $J$ = 8.8 Hz, 2H), 6.69 (d, $J$ = 8.8 Hz, 2H), 3.69 (s, 3H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 153.97, 145.28, 142.11, 131.38, 129.81, 129.66, 129.49, 127.61, 126.92, 126.58, 116.00, 115.72, 56.12. HRMS (ESI) m/z: [M + H]$^+$ calcd for C$_{22}$H$_{20}$N$_{3}$O 342.1606; found 342.1595.

N-(4-Bromophenyl)-2,5-diphenyl-1H-imidazol-5-amine (4e).

![Chemical Structure of 4e](image)
Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4e as off-white solid (0.37 g, yield 95%), mp 138−140 °C. $^1$H NMR (400 MHz, CD$_3$OD): δ 7.94 (d, $J = 7.6$ Hz, 2H), 7.71 (d, $J = 7.6$ Hz, 2H), 7.45 (t, $J = 8.0$ Hz, 2H), 7.39 (d, $J = 7.2$ Hz, 1H), 7.36 (t, $J = 8.0$ Hz, 2H), 7.23 (t, $J = 7.6$ Hz, 1H), 7.20 (d, $J = 7.2$ Hz, 2H), 6.66 (d, $J = 7.2$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): δ 147.59, 145.63, 132.75, 131.23, 129.82, 129.79, 129.58, 127.91, 126.96, 126.62, 116.50, 110.46. HRMS (ESI) m/z: [M + H]$^+$ calcd for C$_{21}$H$_{17}$N$_3$Br 390.0606; found 390.0598.

N-(4-Chlorophenyl)-2,5-diphenyl-1H-imidazol-5-amine (4f).

Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4f as off-white solid (0.33 g, yield 94%), mp 145−147 °C. $^1$H NMR (400 MHz, CD$_3$OD): δ 7.94 (d, $J = 7.6$ Hz, 2H), 7.72 (d, $J = 7.2$ Hz, 2H), 7.45 (t, $J = 7.6$ Hz, 2H), 7.39 (d, $J = 7.2$ Hz, 1H), 7.36 (t, $J = 7.6$ Hz, 2H), 7.23 (t, $J = 7.2$ Hz, 1H), 7.20 (d, $J = 8.0$ Hz, 2H), 6.70 (d, $J = 8.0$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): δ 147.17, 145.63, 132.75, 131.23, 129.83, 129.58, 127.90, 126.97, 126.63, 123.50, 116.01. HRMS (ESI) m/z: [M + H]$^+$ calcd for C$_{21}$H$_{17}$N$_3$Cl 346.1111; found 346.1100.

N-(2-Fluorophenyl)-2,5-diphenyl-1H-imidazol-5-amine (4g).
Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4g as white solid (0.32 g, yield 96%), mp 184−186 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.95 (d, $J = 7.6$ Hz, 2H), 7.74 (d, $J = 7.2$ Hz, 2H), 7.46 (t, $J = 7.6$ Hz, 2H), 7.39 (d, $J = 7.6$ Hz, 1H), 7.34 (t, $J = 8.0$ Hz, 2H), 7.22 (t, $J = 7.2$ Hz, 1H), 7.03 (dd, $J = 12.4$, 8.0 Hz, 1H), 6.85 (t, $J = 8.0$ Hz, 1H), 6.67 (d, $J = 8.0$ Hz, 1H), 6.63 (d, $J = 8.0$ Hz, 1H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 154.15, 151.78, 145.86, 136.35, 136.24, 131.29, 129.88, 129.62, 129.31, 128.03, 126.97, 126.67, 125.45, 119.09, 115.79, 115.61; $^{19}$F NMR (376 MHz, CD$_3$OD): $\delta$ -137.82. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{17}$N$_3$F 330.1407; found 330.1397.

**N-(3-Fluorophenyl)-2,5-diphenyl-1H-imidazol-5-amine (4h).**

Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4h as white solid (0.32 g, yield 98%), mp 187−189 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.95 (d, $J = 7.2$ Hz, 2H), 7.72 (d, $J = 7.2$ Hz, 2H), 7.46 (d, $J = 8.0$ Hz, 2H), 7.40 (d, $J = 7.6$ Hz, 1H), 7.35 (t, $J = 7.2$ Hz, 2H), 7.23 (t, $J = 7.2$ Hz, 1H), 7.08 (q, $J = 7.6$ Hz, 1H),
6.53 (d, $J = 7.6$ Hz, 1H), 6.42 (d, $J = 12.0$ Hz, 1H), 6.36 (t, $J = 7.2$ Hz, 1H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 166.62, 164.22, 150.60, 150.50, 145.70, 131.35, 131.27, 129.85, 129.60, 127.97, 127.01, 126.66, 110.63, 105.27, 105.04, 101.48, 101.23; $^{19}$F NMR (376 MHz, CD$_3$OD): $\delta$ -115.38. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{17}$N$_3$F 330.1407; found 330.1405.

$N$-(4-Fluorophenyl)-2,4-diphenyl-$1H$-imidazol-5-amine (4i).

![Chemical Structure]

Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4i as white solid (0.32 g, yield 97%), mp 150–152 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.94 (d, $J = 7.6$ Hz, 2H), 7.73 (d, $J = 7.2$ Hz, 2H), 7.45 (t, $J = 7.6$ Hz, 2H), 7.38 (d, $J = 7.2$ Hz, 1H), 7.34 (t, $J = 7.6$ Hz, 2H), 7.21 (t, $J = 7.2$ Hz, 1H), 6.84 (d, $J = 8.0$ Hz, 2H), 6.68–6.71 (m, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 158.70, 156.37, 145.51, 144.70, 131.34, 129.84, 129.77, 129.55, 127.81, 126.96, 126.63, 116.38, 116.15, 115.74, 115.66; $^{19}$F NMR (376 MHz, CD$_3$OD): $\delta$ -129.81. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{17}$N$_3$F 330.1407; found 330.1397.

$N$-(4-Bromo-2-fluorophenyl)-2,5-diphenyl-$1H$-imidazol-5-amine (4j).
Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4j as white solid (0.33 g, yield 81%), mp 180–182 °C. \( ^1H \) NMR (400 MHz, CD\(_3\)OD): \( \delta \) 7.94 (d, \( J = 7.6 \) Hz, 2H), 7.72 (d, \( J = 7.2 \) Hz, 2H), 7.46 (t, \( J = 7.2 \) Hz, 2H), 7.40 (d, \( J = 7.2 \) Hz, 1H), 7.36 (t, \( J = 7.6 \) Hz, 2H), 7.24 (t, \( J = 8.0 \) Hz, 2H), 7.00 (d, \( J = 8.4 \) Hz, 1H), 6.58 (t, \( J = 9.6 \) Hz, 1H); \( ^{13}C \) NMR (100 MHz, CD\(_3\)OD): \( \delta \) 153.85, 151.42, 145.94, 136.03, 135.91, 131.25, 129.98, 129.93, 129.73, 128.49, 128.22, 127.04, 126.72, 119.27, 119.05, 116.86, 108.99; \( ^{19}F \) NMR (376 MHz, CD\(_3\)OD): \( \delta \) -134.34 (triplets). HRMS (ESI) \( m/z \): [M + H]\(^+\) calcd for C\(_{21}\)H\(_{16}\)N\(_3\)FBr 408.0512; found 408.0503.

**N-(2-Fluorophenyl)-2,5-diphenyl-1H-imidazol-5-amine (4k).**

Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4k as white solid (0.38 g, yield 93%), mp 147–149 °C. \( ^1H \) NMR (400 MHz, CD\(_3\)OD): \( \delta \) 7.94 (d, \( J = 8.0 \) Hz, 2H), 7.69 (d, \( J = 7.2 \) Hz, 2H), 7.45 (t, \( J = 7.6 \) Hz, 2H), 7.39 (d, \( J = 7.2 \) Hz, 1H), 7.33 (t, \( J = 8.0 \) Hz, 2H), 7.22 (d, \( J = 7.2 \) Hz, 1H), 7.20 (s, 1H), 7.01 (d, \( J = \)
8.8 Hz, 1H), 6.41 (d, \( J = 8.8 \) Hz, 1H); \(^{13}\)C \( \{^1\)H\} NMR (100 MHz, CD\(_3\)OD): \( \delta \) 145.75, 145.61, 133.66, 131.28, 130.33, 129.89, 129.86, 129.60, 127.94, 126.90, 126.63, 126.22, 115.24, 110.67, 17.77. HRMS (ESI) \( m/\ell \): [M + H]\(^+\) calcd for C\(_{22}\)H\(_{19}\)N\(_3\)Br 404.0762; found 404.0753.

\( N\)-\( (3\)-Bromo-5-methylphenyl\)-2,5-diphenyl-1\( H\)-imidazol-5-amine (4l).

\[
\text{Br} \quad \text{NH} \quad \text{N}
\]

Purification by silica gel column chromatography (0 to 20% EtOAc in \( n\)-hexane) afforded 4k as white solid (0.39 g, yield 97%), mp 218–220 °C. \(^1\)H NMR (400 MHz, CD\(_3\)OD): \( \delta \) 7.95 (d, \( J = 7.6 \) Hz, 2H), 7.71 (d, \( J = 7.2 \) Hz, 2H), 7.46 (t, \( J = 7.2 \) Hz, 2H), 7.40 (d, \( J = 7.2 \) Hz, 1H), 7.36 (t, \( J = 8.0 \) Hz, 2H), 7.23 (t, \( J = 7.2 \) Hz, 1H), 6.68 (s, 1H), 6.64 (s, 1H), 6.60 (s, 1H); \(^{13}\)C NMR (100 MHz, CD\(_3\)OD): \( \delta \) 149.84, 145.72, 141.93, 131.28, 129.86, 129.85, 129.62, 127.99, 127.03, 126.68, 123.78, 122.47, 114.73, 114.15, 21.39. HRMS (ESI) \( m/\ell \): [M + H]\(^+\) calcd for C\(_{22}\)H\(_{19}\)N\(_3\)Br 404.0762; found 404.0755.

\( 2,5\)-Diphenyl-\( N\)-\( [4\)-(trifluoromethyl)phenyl\]-1\( H\)-imidazol-5-amine (4m).

\[
\text{F}_3\text{C} \quad \text{NH} \quad \text{N}
\]
Purification by silica gel column chromatography (0 to 20% EtOAc in n-hexane) afforded 4m as white solid (0.35 g, yield 91%), mp 208–210 °C. 1H NMR (400 MHz, CD3OD): δ 7.95 (d, J = 8.0 Hz, 2H), 7.71 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 7.6 Hz, 2H), 7.40–7.33 (m, 5H), 7.24 (t, J = 7.6 Hz, 1H), 6.82 (d, J = 8.4 Hz, 2H); 13C NMR (100 MHz, CD3OD): δ 151.70, 145.85, 131.23, 129.93, 129.90, 129.68, 128.13, 127.84, 127.40, 127.36, 127.05, 126.69, 125.16, 114.21; 19F NMR (376 MHz, CD3OD): δ -62.55. HRMS (ESI) m/z: [M + H]+ calcd for C22H17N3F3 380.1375; found 380.1356.

Methyl 4-[(2,5-diphenyl-1H-imidazol-5-yl)amino]benzoate (4n).

Purification by silica gel column chromatography (0 to 25% EtOAc in n-hexane) afforded 4n as white solid (0.35 g, yield 95%), mp 140–142 °C. 1H NMR (400 MHz, CD3OD): δ 7.95 (d, J = 7.6 Hz, 2H), 7.79 (d, J = 8.8 Hz, 2H), 7.70 (d, J = 7.2 Hz, 2H), 7.46 (t, J = 7.2 Hz, 2H), 7.40 (d, J = 7.2 Hz, 1H), 7.30 (m, 5H), 7.23 (t, J = 7.2 Hz, 2H), 6.76 (d, J = 7.2 Hz, 2H), 3.81 (s, 3H); 13C NMR (100 MHz, CD3OD): δ 169.12, 153.21, 145.96, 132.42, 131.25, 129.99, 129.95, 129.72, 128.21, 127.12, 126.74, 119.99, 113.90, 52.08. HRMS (ESI) m/z: [M + H]+ calcd for C23H20N3O2 370.1556; found 370.1545.

4-[(2,5-Diphenyl-1H-imidazol-5-yl)amino]benzonitrile (4o).
Purification by silica gel column chromatography (0 to 25% EtOAc in \textit{n}-hexane) afforded 4o as white solid (0.23 g, yield 69\%), mp 129–131 °C. \textsuperscript{1}H NMR (400 MHz, CD\textsubscript{3}OD): \(\delta\) 7.95 (d, \(J = 7.6\) Hz, 2H), 7.68 (d, \(J = 7.6\) Hz, 2H), 7.48 (t, \(J = 7.2\) Hz, 2H), 7.44 (d, \(J = 7.6\) Hz, 2H), 7.39 (d, \(J = 7.2\) Hz, 1H), 7.36 (t, \(J = 8.0\) Hz, 2H), 7.25 (t, \(J = 7.2\) Hz, 1H), 6.68 (d, \(J = 7.2\) Hz, 2H); \textsuperscript{13}C NMR (100 MHz, CD\textsubscript{3}OD): \(\delta\) 152.76, 146.12, 134.69, 131.19, 130.06, 129.96, 129.78, 128.35, 127.14, 126.75, 121.23, 114.83, 100.26. HRMS (ESI) \(m/z\): [M + H]\textsuperscript{+} calcd for C\textsubscript{22}H\textsubscript{17}N\textsubscript{4} 337.1453; found 337.1442.

\textit{N}-(4-Nitrophenyl)-2,5-diphenyl-1\textit{H}-imidazol-5-amine (4p).

Purification by silica gel column chromatography (0 to 20% EtOAc in \textit{n}-hexane) afforded 4p as white solid (0.15 g, yield 41\%), mp 217–219 °C. \textsuperscript{1}H NMR (400 MHz, CD\textsubscript{3}OD): \(\delta\) 8.04 (d, \(J = 8.8\) Hz, 2H), 7.96 (d, \(J = 7.6\) Hz, 2H), 7.68 (t, \(J = 7.6\) Hz, 2H), 7.46 (t, \(J = 7.2\) Hz, 2H), 7.40 (d, \(J = 7.2\) Hz, 1H), 7.36 (t, \(J = 7.6\) Hz, 2H), 7.25 (t, \(J = 7.6\) Hz, 1H), 6.91 (d, \(J = 8.8\) Hz, 2H); \textsuperscript{13}C NMR (100 MHz, CD\textsubscript{3}OD): \(\delta\) 154.68, 146.19, 139.86, 131.07,
130.07, 129.92, 129.78, 128.42, 127.15, 126.99, 126.73, 113.74. HRMS (ESI) m/z: [M + H]⁺ calcd for C₂₁H₁₇N₄O₂ 357.1352; found 357.1348.

\[ \text{N-(2,5-Diphenyl-1H-imidazol-5-yl)-1-methyl-1H-indazol-5-amine (4q).} \]

\[
\text{Purification by silica gel column chromatography (0 to 35\% EtOAc in n-hexane) afforded 4p as white solid (0.20 g, yield 55\%), mp 114−116 °C.} \\
\text{\( ^1 \)H NMR (400 MHz, CD₃OD): } \delta 7.94 (s, 1H), 7.92 (s, 1H), 7.73 (d, \( J = 8.4 \) Hz, 2H), 7.44 (t, \( J = 7.6 \) Hz, 2H), 7.36 (t, \( J = 8.4 \) Hz, 1H), 7.32 (t, \( J = 8.4 \) Hz, 2H), 7.19 (t, \( J = 7.6 \) Hz, 1H), 6.73 (d, \( J = 8.8 \) Hz, 2H), 6.68 (d, \( J = 8.8 \) Hz, 2H), 3.68 (s,3H); \text{\( ^{13} \)C NMR (100 MHz, CD₃OD): } \delta 145.52, 142.92, 136.94, 132.30, 131.39, 129.95, 129.78, 128.68, 127.75, 126.89, 126.57, 126.98, 119.55, 110.94, 102.36, 35.35 . \text{HRMS (ESI) m/z: [M + H]⁺ calcd for C₂₃H₂₀N₅ 366.1719; found 366.1707.} \\
\]

\[ \text{N-(4-Bromophenyl)-2-phenyl-5-(p-tolyl)-1H-imidazol-5-amine (4r).} \]

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\text{S14}
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Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4r as white solid (0.37 g, yield 92%), mp 109−111 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.92 (d, $J = 7.6$ Hz, 2H), 7.69 (d, $J = 7.6$ Hz, 2H), 7.42 (t, $J = 7.2$ Hz, 2H), 7.35 (t, $J = 7.2$ Hz, 1H), 7.18 (d, $J = 7.6$ Hz, 2H), 7.14 (d, $J = 8.0$ Hz, 2H), 6.63 (d, $J = 8.4$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 147.72, 145.35, 137.89, 132.74, 131.29, 130.22, 130.12, 129.82, 129.72, 126.92, 126.57, 11.46, 110.34, 21.24. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{22}$H$_{19}$N$_3$Br 404.0762; found 404.0755.

$N$-(4-Bromophenyl)-5-(4-methoxyphenyl)-2-phenyl-$1H$-imidazol-5-amine (4s).

Purification by silica gel column chromatography (0 to 13% EtOAc in n-hexane) afforded 4s as off white solid (0.31 g, yield 75%), mp 190−192 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.92 (d, $J = 8.4$ Hz, 2H), 7.63 (d, $J = 7.6$ Hz, 2H), 7.44 (t, $J = 7.6$ Hz, 2H), 7.56 (d, $J = 8.4$ Hz, 1H), 7.54 (d, $J = 8.4$ Hz, 1H), 7.44 (t, $J = 7.6$ Hz, 2H), 7.37 (t, $J = 7.6$ Hz, 1H), 7.19 (d, $J = 8.4$ Hz, 2H), 6.91 (d, $J = 8.4$ Hz, 2H), 6.63 (d, $J = 8.4$ Hz, 2H), 3.78 (s, 3H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 160.23, 147.88, 145.11, 132.75, 131.34, 129.83, 129.66, 128.40, 126.51, 116.41, 115.03, 114.30, 110.30, 55.68. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{22}$H$_{19}$N$_3$OBr 420.0712; found 420.0698.
2-(Benzofuranyl)-N-(4-bromophenyl)-2-phenyl-6-methylimidazole (4v).

Purification by silica gel column chromatography (0 to 15% EtOAc in n-hexane) afforded 4v as white solid (0.27 g, yield 66%), mp 101–103 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.94 (d, $J = 7.6$ Hz, 2H), 7.44 (t, $J = 7.6$ Hz, 2H), 7.37 (t, $J = 7.2$ Hz, 1H), 7.31 (d, $J = 7.6$ Hz, 1H), 7.30 (s, 1H), 7.25 (t, $J = 8.4$ Hz, 1H), 7.20 (d, $J = 8.8$ Hz, 2H), 6.77 (d, $J = 8.4$ Hz, 1H), 6.65 (d, $J = 8.8$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 161.26, 147.60, 145.62, 132.80, 131.23, 130.60, 129.85, 126.67, 119.22, 116.50, 1113.99, 112.09, 110.47, 55.52. HRMS (ESI) m/z: [M + H]$^+$ calcd for C$_{22}$H$_{19}$N$_3$OBr 420.0712; found 420.0692.

2-(Benzofuran-2-yl)-N-(4-bromophenyl)-2-phenyl-1H-imidazole (4w).

Purification by silica gel column chromatography (0 to 15% EtOAc in n-hexane) afforded 4w as white solid (0.27 g, yield 66%), mp 101–103 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.94 (d, $J = 7.6$ Hz, 2H), 7.44 (t, $J = 7.6$ Hz, 2H), 7.37 (t, $J = 7.2$ Hz, 1H), 7.31 (d, $J = 7.6$ Hz, 1H), 7.30 (s, 1H), 7.25 (t, $J = 8.4$ Hz, 1H), 7.20 (d, $J = 8.8$ Hz, 2H), 6.77 (d, $J = 8.4$ Hz, 1H), 6.65 (d, $J = 8.8$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 161.26, 147.60, 145.62, 132.80, 131.23, 130.60, 129.85, 126.67, 119.22, 116.50, 1113.99, 112.09, 110.47, 55.52. HRMS (ESI) m/z: [M + H]$^+$ calcd for C$_{22}$H$_{19}$N$_3$OBr 420.0712; found 420.0692.
Purification by silica gel column chromatography (0 to 25% EtOAc in n-hexane) afforded 4u as white solid (0.30 g, yield 69%), mp 117−119 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.91 (d, $J = 7.2$ Hz, 2H), 7.44 (t, $J = 7.4$ Hz, 2H), 7.39 (t, $J = 7.6$ Hz, 2H), 7.24−7.19 (m, 4H), 6.82 (d, $J = 8.4$ Hz, 1H), 6.63 (d, $J = 8.4$ Hz, 2H), 5.93 (s, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 149.33, 148.11, 147.73, 145.20, 142.02, 132.79, 131.29, 129.85, 129.75, 129.01, 126.56, 126.22, 120.87, 116.44, 110.47, 109.36, 107.58, 102.42. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{22}$H$_{17}$N$_3$O$_2$Br 434.0504; found 434.0498.

$N,N$-Bis(4-bromophenyl)-2-phenyl-1H-imidazol-5-amine (4v).

Purification by silica gel column chromatography (0 to 14% EtOAc in n-hexane) afforded 4v as off white solid (0.30 g, yield 64%), mp 176−178 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.93 (d, $J = 7.6$ Hz, 2H), 7.65 (d, $J = 8.4$ Hz, 2H), 7.49 (d, $J = 8.4$ Hz, 2H), 7.43 (t, $J = 8.0$ Hz, 2H), 7.39 (t, $J = 8.0$ Hz, 1H), 7.22 (d, $J = 8.4$ Hz, 2H), 6.65 (d, $J = 8.4$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 147.27, 145.98, 132.85, 132.66, 131.11, 129.95, 129.86, 128.55, 126.65, 121.42, 116.55, 110.73. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{16}$N$_3$Br$_2$ 467.9711; found 467.9702.

$5$-(3-Bromophenyl)-$N$-(4-bromophenyl)-2-phenyl-1H-imidazol-5-amine (4w).
Purification by silica gel column chromatography (0 to 20% EtOAc in n-hexane) afforded **4w** as off white solid (0.32 g, yield 69%), mp 96–98 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.95 (s, 1H), 7.94 (d, $J = 8.0$ Hz, 2H), 7.71 (d, $J = 8.0$ Hz, 1H), 7.46 (t, $J = 8.0$ Hz, 2H), 7.41 (t, $J = 7.2$ Hz, 1H), 7.36 (d, $J = 7.0$ Hz, 1H), 7.26 (d, $J = 8.0$ Hz, 1H), 7.22 (d, $J = 8.8$ Hz, 2H), 6.66 (d, $J = 8.8$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 147.22, 146.28, 132.87, 131.30, 131.10, 130.56, 130.01, 129.88, 129.59, 129.56, 126.71, 125.48, 123.66, 116.61, 110.78. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{16}$N$_3$Br$_2$ 467.9711; found 467.9703.

**N-(4-Bromophenyl)-5-(4-chlorophenyl)-2-phenyl-1H-imidazol-5-amine (4x).**

Purification by silica gel column chromatography (0 to 20% EtOAc in n-hexane) afforded **4x** as white solid (0.40 g, yield 94%), mp 162–164 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.93 (d, $J = 7.6$ Hz, 2H), 7.71 (t, $J = 8.0$ Hz, 2H), 7.45 (t, $J = 7.2$ Hz, 2H), 7.39 (t, $J = 7.2$ Hz, 1H), 7.31 (d, $J = 8.8$ Hz, 2H), 7.21 (d, $J = 8.8$ Hz, 2H), 6.65 (d, $J = 8.8$ Hz, 2H);
$^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 147.35, 145.97, 133.48, 132.86, 131.14, 129.95, 129.87, 129.68, 128.31, 126.66, 116.56, 110.71. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{16}$N$_3$ClBr 424.0216; found 424.0208.

$N$-(4-Bromophenyl)-5-(4-fluorophenyl)-2-phenyl-1$H$-imidazol-5-amine (4y).

Purification by silica gel column chromatography (0 to 15% EtOAc in $n$-hexane) afforded 4y as white solid (0.40 g, yield 97%), mp 123−125 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.93 (d, $J =$ 7.6 Hz, 2H), 7.73 (t, $J =$ 6.0 Hz, 2H), 7.45 (t, $J =$ 7.2 Hz, 2H), 7.38 (t, $J =$ 7.2 Hz, 1H), 7.21 (d, $J =$ 8.8 Hz, 2H), 7.08 (t, $J =$ 8.8 Hz, 2H), 6.64 (d, $J =$ 8.8 Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 164.43, 161.99, 147.66, 145.72, 132.87, 131.27, 130.30, 129.91, 129.04, 128.96, 126.65, 116.51, 116.39, 116.28, 110.58; $^{19}$F NMR (376 MHz, CD$_3$OD): $\delta$ -126.85. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{16}$N$_3$BrF 408.0512; found 408.0502.

$N$-(4-Bromophenyl)-5-(3-fluorophenyl)-2-phenyl-1$H$-imidazol-5-amine (4z).
Purification by silica gel column chromatography (0 to 12% EtOAc in n-hexane) afforded 4z as off white solid (0.22 g, yield 55%), mp 106–108 °C. \(^1\)H NMR (400 MHz, CD\(_3\)OD): \(\delta\) 7.94 (d, \(J = 7.6\) Hz, 2H), 7.56 (d, \(J = 7.6\) Hz, 1H), 7.51 (d, \(J = 10.8\) Hz, 1H), 7.45 (t, \(J = 7.2\) Hz, 2H), 7.40 (d, \(J = 7.2\) Hz, 1H), 7.31 (q, \(J = 7.6\) Hz, 1H), 7.22 (d, \(J = 8.4\) Hz, 2H), 6.94 (t, \(J = 8.0\) Hz, 1H), 6.66 (d, \(J = 8.4\) Hz, 2H); \(^13\)C NMR (100 MHz, CD\(_3\)OD): \(\delta\) 165.65, 163.23, 147.29, 132.87, 131.38, 131.30, 131.11, 130.02, 129.89, 126.72, 122.60, 116.56, 114.42, 114.21, 113.49, 113.26, 110.76; \(^19\)F NMR (376 MHz, CD\(_3\)OD): \(\delta\) -114.84. HRMS (ESI) \(m/z\): [M + H]\(^+\) calcd for C\(_{21}\)H\(_{16}\)N\(_3\)Br F 408.0512; found 408.0499.

N-(4-Bromophenyl)-5-(3,4-difluorophenyl)-2-phenyl-1H-imidazol-5-amine (4aa).

Purification by silica gel column chromatography (0 to 15% EtOAc in n-hexane) afforded 4aa as white solid (0.41 g, yield 96%), mp 182–184 °C. \(^1\)H NMR (400 MHz,
CD$_3$OD): $\delta$ 7.93 (d, $J = 7.6$ Hz, 2H), 7.65 (t, $J = 9.6$ Hz, 1H), 7.53 (brs, 1H), 7.45 (t, $J = 7.6$ Hz, 2H), 7.39 (t, $J = 7.6$ Hz, 1H), 7.26–7.20 (m, 3H), 6.65 (d, $J = 8.4$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 152.83, 152.70, 151.57, 151.44, 150.38, 150.25, 149.11, 148.98, 147.16, 146.01, 132.91, 131.05, 130.00, 129.87, 126.65, 123.38, 123.34, 123.28, 118.50, 118.32, 116.54, 115.75, 115.56, 110.92; $^{19}$F NMR (376 MHz, CD$_3$OD): $\delta$ -140.18, -142.51. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{15}$N$_3$BrF$_2$ 426.0417; found 426.0406.

$N$-(4-Bromophenyl)-5-(2,4-difluorophenyl)-2-phenyl-1H-imidazol-5-amine (4ab).

Purification by silica gel column chromatography (0 to 15% EtOAc in $n$-hexane) afforded 4ab as white solid (0.31 g, yield 73%), mp 166–168 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.90 (d, $J = 8.0$ Hz, 2H), 7.56 (q, $J = 8.4$ Hz, 1H), 7.44 (t, $J = 7.2$ Hz, 2H), 7.37 (t, $J = 7.2$ Hz, 1H), 7.18 (d, $J = 8.0$ Hz, 2H), 7.03 (brs, 1H), 6.97 (t, $J = 7.6$ Hz, 1H), 6.69 (d, $J = 6.0$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 163.73, 163.62, 161.26, 161.14, 145.99, 144.55, 131.25, 131.06, 129.75, 128.48, 125.10, 115.19, 111.22, 111.03, 109.14, 103.93, 103.67, 103.61; $^{19}$F NMR (376 MHz, CD$_3$OD): $\delta$ -111.40, -112.20. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{21}$H$_{15}$N$_3$F$_2$Br 426.0417; found 426.0410.

$N$-(4-Bromophenyl)-2-phenyl-5-(4-(trifluoromethyl)phenyl)-1H-imidazol-5-amine (4ac).
Purification by silica gel column chromatography (0 to 15% EtOAc in n-hexane) afforded 4ac as white solid (0.43 g, yield 93%), mp 124–126 °C. $^1$H NMR (400 MHz, CD$_3$OD): δ 7.94 (t, $J = 7.6$ Hz, 4H), 7.64 (d, $J = 7.6$ Hz, 2H), 7.47 (t, $J = 7.2$ Hz, 2H), 7.40 (t, $J = 7.2$ Hz, 1H), 7.24 (d, $J = 7.6$ Hz, 2H), 6.70 (d, $J = 7.6$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): δ 147.06, 146.54, 132.93, 131.06, 130.14, 129.91, 129.39, 129.07, 127.10, 126.98, 126.78, 126.48, 126.44, 124.40, 116.69, 110.97; $^{19}$F NMR (376 MHz, CD$_3$OD): δ -63.99. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{22}$H$_{16}$N$_3$F$_3$Br 458.0480; found 458.0471.

$N$-(4-Bromophenyl)-2-phenyl-5-(2-(trifluoromethyl)phenyl)-1H-imidazol-5-amine (4ad).

Purification by silica gel column chromatography (0 to 25% EtOAc in n-hexane) afforded 4ad as white solid (0.17 g, yield 37%), mp 208–210 °C. $^1$H NMR (400 MHz, CD$_3$OD): δ 7.87 (d, $J = 8.4$ Hz, 2H), 7.79 (d, $J = 8.4$ Hz, 1H), 7.62 (d, $J = 8.8$ Hz, 1H), 7.56 (d, $J = 8.4$ Hz, 1H), 7.54 (d, $J = 8.4$ Hz, 1H), 7.44 (t, $J = 7.6$ Hz, 2H), 7.37 (t, $J = 7.6$ Hz, 1H), 7.16 (d, $J = 8.4$ Hz, 2H), 6.69 (d, $J = 8.4$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): δ 147.78,
145.25, 134.53, 132.97, 132.53, 131.27, 131.22, 130.92, 129.98, 129.91, 129.80, 127.48, 127.42, 127.37, 127.32, 126.83, 126.39, 124.12, 116.64, 110.38; $^{19}$F NMR (376 MHz, CD$_3$OD): $\delta$ -60.53. HRMS (ESI) $m/\epsilon$: [M + H]$^+$ calcd for C$_{22}$H$_{16}$N$_3$F$_3$Br 458.0480; found 458.0467.

$N$-(4-Bromophenyl)-2-phenyl-5-(thiophen-2-yl)-1H-imidazol-5-amine (4ae).

![Chemical structure](image)

Purification by silica gel column chromatography (0 to 17% EtOAc in $n$-hexane) afforded 4ae as white solid (0.26 g, yield 67%), mp 140–143 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.93 (d, $J = 7.6$ Hz, 2H), 7.45 (t, $J = 7.2$ Hz, 2H), 7.39 (d, $J = 7.2$ Hz, 1H), 7.38 (d, $J = 7.2$ Hz, 1H), 7.29 (d, $J = 4.8$ Hz, 1H), 7.21 (d, $J = 8.8$ Hz, 2H), 7.02 (t, $J = 4.8$ Hz, 1H), 6.64 (d, $J = 8.8$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 147.48, 145.61, 132.80, 131.15, 129.96, 129.92, 129.75, 129.68, 127.98, 126.66, 125.63, 124.16, 116.55, 110.64. HRMS (ESI) $m/\epsilon$: [M + H]$^+$ calcd for C$_{19}$H$_{15}$N$_3$SBr 396.0170; found 396.0164.

$N$-(4-Bromophenyl)-5-(naphthalen-2-yl)-2-phenyl-1H-imidazol-5-amine (4af).
Purification by silica gel column chromatography (0 to 10% EtOAc in n-hexane) afforded 4af as off white solid (0.25 g, yield 58%), mp 180–183 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 8.18 (brs, 1H), 7.98 (d, $J = 7.2$ Hz, 2H), 7.89 (d, $J = 7.6$ Hz, 1H), 7.80 (t, $J = 7.6$ Hz, 3H), 7.50–7.36 (m, 5H), 7.22 (d, $J = 8.8$ Hz, 2H), 6.72 (t, $J = 8.8$ Hz, 2H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 147.69, 135.03, 133.80, 132.87, 131.31, 129.94, 129.24, 129.20, 129.03, 128.66, 127.41, 126.94, 126.74, 125.32, 125.23, 116.68. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{25}$H$_{19}$N$_3$Br 440.0762; found 440.0747.

$N$-(4-Bromophenyl)-5-(6-methoxynaphthalen-2-yl)-2-phenyl-1H-imidazol-5-amine (4ag).

Purification by silica gel column chromatography (0 to 20% EtOAc in n-hexane) afforded 4ag as off white solid (0.37 g, yield 80 %), mp 207–209 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 8.09 (s, 1H), 7.97 (d, $J = 8.0$ Hz, 2H), 7.83 (d, $J = 8.0$ Hz, 1H), 7.70 (d, $J = 8.4$ Hz, 1H), 7.69 (d, $J = 8.8$ Hz, 1H), 7.46 (t, $J = 8.8$ Hz, 2H), 7.39 (t, $J = 7.6$ Hz, 1H), 7.21 (t, $J$
= 8.8 Hz, 2H), 7.19 (s, 1H), 7.11 (d, \( J = 8.8 \text{ Hz}, 1H \)), 6.70 (d, \( J = 8.4 \text{ Hz}, 2H \)), 3.88 (s, 3H);

\(^{13}\)C NMR (100 MHz, CD\(_3\)OD): \( \delta \) 161.80, 150.29, 148.14, 137.53, 135.31, 133.83, 132.97, 132.87, 132.39, 132.31, 130.62, 129.14, 128.22, 127.78, 122.65, 119.09, 112.95, 109.20, 58.25

HRMS (ESI) m/z: [M + H]\(^+\) calcd for C\(_{26}\)H\(_{21}\)N\(_3\)OBr 470.0868; found 470.0866.

\( N\)-(4-Bromophenyl)-5-phenyl-2-(\( p \)-tolyl)-1\( H \)-imidazol-5-amine (4ah).

\[
\text{\begin{tikzpicture}
\draw[thick] (0,0) -- (1,0) -- (1,1) -- (0,1) -- cycle;
\draw[thick] (1,0) -- (2,0);
\draw[thick] (1,1) -- (2,1);
\draw[thick] (2,0) -- (2,1);
\draw[thick] (0,1) -- (1,2);
\fill[white] (2,0.5) circle (0.25);
\fill[white] (2,1.5) circle (0.25);
\fill[white] (1,0.5) circle (0.25);
\fill[white] (1,1.5) circle (0.25);
\end{tikzpicture}}\]

Purification by silica gel column chromatography (0 to 13% EtOAc in \( n \)-hexane) afforded 4ah as off white solid (0.38 g, yield 94%), mp 188–190 \( ^\circ \)C. \( ^1\)H NMR (400 MHz, CD\(_3\)OD): \( \delta \) 7.82 (d, \( J = 8.4 \text{ Hz}, 2H \)), 7.70 (d, \( J = 7.2 \text{ Hz}, 2H \)), 7.34 (t, \( J = 7.6 \text{ Hz}, 2H \)), 7.27 (d, \( J = 8.0 \text{ Hz}, 2H \)), 7.22 (d, \( J = 7.2 \text{ Hz}, 1H \)), 7.19 (d, \( J = 8.4 \text{ Hz}, 2H \)), 6.65 (d, \( J = 8.4 \text{ Hz}, 2H \)), 2.38 (s, 3H); \( ^{13}\)C NMR (100 MHz, CD\(_3\)OD): \( \delta \) 147.72, 145.89, 140.09, 132.77, 131.73, 130.47, 129.59, 128.53, 127.87, 126.93, 126.67, 126.65, 116.48, 110.40, 21.33.

HRMS (ESI) m/z: [M + H]\(^+\) calcd for C\(_{22}\)H\(_{19}\)N\(_3\)Br 404.0762; found 404.0747.

\( N\)-(4-Bromophenyl)-2-(4-methoxyphenyl)-5-phenyl-1\( H \)-imidazol-5-amine (4ai).

\[
\text{\begin{tikzpicture}
\draw[thick] (0,0) -- (1,0) -- (1,1) -- (0,1) -- cycle;
\draw[thick] (1,0) -- (2,0);
\draw[thick] (1,1) -- (2,1);
\draw[thick] (2,0) -- (2,1);
\draw[thick] (0,1) -- (1,2);
\fill[white] (2,0.5) circle (0.25);
\fill[white] (2,1.5) circle (0.25);
\fill[white] (1,0.5) circle (0.25);
\fill[white] (1,1.5) circle (0.25);
\end{tikzpicture}}\]
Purification by silica gel column chromatography (0 to 25% EtOAc in n-hexane) afforded 4ai as white solid (0.38 g, yield 90%), mp 215–217 °C. 1H NMR (400 MHz, CD3OD): δ 7.87 (d, J = 8.8 Hz, 2H), 7.70 (d, J = 7.2 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.22 (d, J = 7.2 Hz, 1H), 7.20 (d, J = 7.2 Hz, 2H), 7.01 (d, J = 8.8 Hz, 2H), 6.65 (d, J = 8.4 Hz, 2H); 13C NMR (100 MHz, CD3OD): δ 161.80, 147.78, 145.90, 132.76, 129.59, 128.19, 127.78, 126.84, 123.98, 116.47, 115.22, 110.34, 55.81. HRMS (ESI) m/z: [M + H]+ calcd for C22H19N3OBr 420.0712; found 420.0699.

N,N2-Bis(4-bromophenyl)-5-phenyl-1H-imidazol-5-amine (4aj).

Purification by silica gel column chromatography (0 to 11% EtOAc in n-hexane) afforded 4aj as white solid (0.37 g, yield 80%), mp 213–215 °C. 1H NMR (400 MHz, CD3OD): δ 7.84 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 7.2 Hz, 2H), 7.60 (d, J = 8.4 Hz, 2H), 7.34 (t, J = 7.6 Hz, 2H), 7.24 (d, J = 7.2 Hz, 1H), 7.20 (d, J = 7.6 Hz, 2H), 6.66 (d, J = 7.6 Hz, 2H); 13C NMR (100 MHz, CD3OD): δ 147.48, 144.42,132.99, 132.77, 130.32, 129.62, 128.25, 128.05, 126.99, 123.66, 116.53, 110.54. HRMS (ESI) m/z calcd for C21H16N3Br2, [M + H]+ 467.9711; found: 467.9702.

N-(4-Bromophenyl)-2-(4-chlorophenyl)-5-phenyl-1H-imidazol-5-amine (4ak).
Purification by silica gel column chromatography (0 to 20% EtOAc in n-hexane) afforded 4ak as white solid (0.36 g, yield 83%), mp 205–207 °C. \( ^1H \) NMR (400 MHz, CD$_3$OD): \( \delta \) 7.92 (d, \( J = 8.4 \) Hz, 2H), 7.71 (d, \( J = 7.2 \) Hz, 2H), 7.46 (d, \( J = 8.4 \) Hz, 2H), 7.35 (t, \( J = 7.6 \) Hz, 2H), 7.24 (d, \( J = 7.2 \) Hz, 1H), 7.20 (d, \( J = 7.6 \) Hz, 2H), 6.66 (d, \( J = 8.4 \) Hz, 2H); \( ^{13}C \) NMR (100 MHz, CD$_3$OD): \( \delta \) 147.55, 144.42, 135.60, 132.78, 130.01, 129.64, 128.06, 127.00, 116.52, 110.53. HRMS (ESI) \( m/z \): [M + H]$^+$ calcd for C$_{21}$H$_{16}$N$_3$ClBr 424.0216; found 424.0199.

\( \text{N-(4-Bromophenyl)-2-(4-fluorophenyl)-5-phenyl-1H-imidazol-5-amine (4al).} \)

Purification by silica gel column chromatography (0 to 13% EtOAc in n-hexane) afforded 4al as white solid (0.37 g, yield 90%), mp 174–175 °C. \( ^1H \) NMR (400 MHz, CD$_3$OD): \( \delta \) 7.96 (dd, \( J = 8.8, 5.6 \) Hz, 2H), 7.71 (d, \( J = 8.0 \) Hz, 2H), 7.35 (t, \( J = 8.0 \) Hz, 2H), 7.25–7.17 (m, 5H), 6.66 (d, \( J = 8.4 \) Hz, 2H); \( ^{13}C \) NMR (100 MHz, CD$_3$OD): \( \delta \) 165.70, 163.24, 147.63, 144.76, 132.78, 129.62, 128.82, 128.73, 127.98, 127.78, 126.94, 116.82, 116.60,
116.49, 110.47; \textsuperscript{19}F NMR (376 MHz, CD\textsubscript{3}OD): \(\delta\) -114.66. HRMS (ESI) \(m/z\): [M + H]\(^+\) calcd for C\textsubscript{21}H\textsubscript{16}N\textsubscript{3}BrF 408.0512; found 408.0497.

\textit{N-}(4-Bromophenyl)-5-phenyl-2-[4-(trifluoromethyl)phenyl]-1\textit{H}-imidazol-5-amine (4am).

\[ \text{Aromatic structure image} \]

Purification by silica gel column chromatography (0 to 25\% EtOAc in \textit{n}-hexane) afforded 4am as white solid (0.43 g, yield 93\%), mp 215–217 °C. \textsuperscript{1}H NMR (400 MHz, CD\textsubscript{3}OD): \(\delta\) 8.12 (d, \(J = 8.0\) Hz, 2H), 7.75 (d, \(J = 8.0\) Hz, 2H), 7.73 (d, \(J = 8.0\) Hz, 2H), 7.36 (t, \(J = 7.6\) Hz, 2H), 7.25 (t, \(J = 7.2\) Hz, 1H), 7.21 (d, \(J = 8.4\) Hz, 2H), 6.68 (d, \(J = 8.4\) Hz, 2H); \textsuperscript{13}C NMR (100 MHz, CD\textsubscript{3}OD): \(\delta\) 147.44, 143.79, 134.82, 132.81, 131.32, 131.00, 129.68, 128.25, 127.13, 126.91, 126.83, 126.80, 124.26, 116.59, 110.63; \textsuperscript{19}F NMR (376 MHz, CD\textsubscript{3}OD): \(\delta\) -64.20. HRMS (ESI) \(m/z\): [M + H]\(^+\) calcd for C\textsubscript{22}H\textsubscript{16}N\textsubscript{3}BrF\textsubscript{3} 458.0480; found 458.0473.

\textit{N-}(4-Bromophenyl)-2-(4-nitrophenyl)-5-phenyl-1\textit{H}-imidazol-5-amine (4an).

\[ \text{Aromatic structure image} \]
Purification by silica gel column chromatography (0 to 13% EtOAc in n-hexane) afforded 4an as brown solid (0.15 g, yield 35%), mp 236–239 °C. \(^1\)H NMR (400 MHz, CD\(_3\)OD): \(\delta\) 8.32 (d, \(J = 8.4\) Hz, 2H), 8.16 (d, \(J = 8.4\) Hz, 2H), 7.74 (d, \(J = 8.0\) Hz, 2H), 7.38 (t, \(J = 8.0\) Hz, 2H), 7.27 (t, \(J = 8.0\) Hz, 2H), 7.22 (d, \(J = 8.4\) Hz, 2H), 6.70 (d, \(J = 8.4\) Hz, 2H); \(^1\)C NMR (100 MHz, CD\(_3\)OD): \(\delta\) 146.45, 144.97, 140.69, 134.75, 130.57, 127.48, 126.18, 124.98, 124.75, 122.95, 114.44, 108.52. HRMS (ESI) \(m/z\): [M + H]+ calcd for C\(_{21}\)H\(_{16}\)N\(_4\)O\(_2\)Br 435.0457; found 435.0438.

\(N\)-(4-Bromophenyl)-5-phenyl-2-(pyridin-2-yl)-1\(H\)-imidazol-5-amine (4ao).

Purification by silica gel column chromatography (0 to 40% EtOAc in n-hexane) afforded 4ao as brown solid (0.11 g, yield 30%), mp 155–157 °C. \(^1\)H NMR (400 MHz, CD\(_3\)OD): \(\delta\) 8.63 (d, \(J = 4.0\) Hz, 1H), 8.04 (d, \(J = 7.6\) Hz, 1H), 7.86 (td, \(J = 8.0\) Hz, 1.6 Hz, 1H), 7.74 (d, \(J = 7.6\) Hz, 2H), 7.38–7.34 (m, 3H), 7.24 (t, \(J = 7.6\) Hz, 1H), 7.21 (d, \(J = 8.8\) Hz, 2H), 6.68 (d, \(J = 8.8\) Hz, 2H); \(^1\)C NMR (100 MHz, CD\(_3\)OD): \(\delta\) 149.00, 147.96, 146.05, 142.99, 137.14, 131.46, 128.37, 126.92, 125.77, 123.20, 119.83, 115.29, 115.12, 109.18. HRMS (ESI) \(m/z\): [M + H]+ calcd for C\(_{20}\)H\(_{16}\)N\(_4\)Br 391.0558; found 391.0545.

\(N\)-(4-Bromophenyl)-5-phenyl-2-(1\(H\)-pyrazol-1-yl)-1\(H\)-imidazol-5-amine (4ap).
Purification by silica gel column chromatography (0 to 20% EtOAc in n-hexane) afforded 4ap as white solid (0.12 g, yield 30%), mp 236–239 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 8.25 (d, $J = 2.0$ Hz, 1H), 7.76 (s, 1H), 7.70 (d, $J = 7.6$ Hz, 2H), 7.34 (d, $J = 7.6$ Hz, 2H), 7.24–7.20 (m, 3H), 6.67 (d, $J = 8.8$ Hz, 2H), 6.53 (t, $J = 2.0$ Hz, 1H); $^{13}$C NMR (100 MHz, CD$_3$OD): $\delta$ 146.02, 141.56, 138.97, 131.41, 128.17, 127.68, 126.54, 125.46, 115.15, 109.31, 109.45. HRMS (ESI) $m/z$: [M + H]$^+$ calcd for C$_{18}$H$_{15}$N$_5$Br 380.0511; found 380.0502.

Tert-butyl [5-[(4-bromophenyl)amino]-4-phenyl-1H-imidazol-2-yl]carbamate (4aq).

Purification by silica gel column chromatography (0 to 35% EtOAc in n-hexane) afforded 4aq as white solid (0.24 g, yield 63%), mp 236–239 °C. $^1$H NMR (400 MHz, CD$_3$OD): $\delta$ 7.75 (d, $J = 7.2$ Hz, 2H), 7.29–7.23 (m, 4H), 7.20 (t, $J = 7.2$ Hz, 1H), 6.51 (d, $J = 8.8$ Hz, 2H), 1.35 (s, 9H); $^{13}$C NMR (150 MHz, CD$_3$OD): $\delta$ 149.76, 148.89, 145.30, 133.42,
132.50, 132.09, 128.30, 127.37, 126.49, 117.13, 115.49, 111.26, 85.73, 27.82. HRMS (ESI) m/z: [M + H]^+ calcd for C_{20}H_{22}N_{4}O_{2}Br 429.0926; found 429.0923.

(2-Bromophenyl)(4-phenyl-2-(phenylamino)-5-(p-tolylamino)-1H-imidazol-1-yl)methanone (5a).

![Chemical structure image]

TEA (0.76 g, 2.30 mmol) and 4-DMAP (0.02 g, 0.15 mmol) were added to a solution of 4a (0.25 g, 0.77 mmol) in DCM: THF (4: 1) (15 mL) at 0 °C and stirred for 30 minutes. To this mixture 2-bromobenzoyl chloride (0.18 g, 0.85 mmol) was added drop wise and stirred for 16h slowly raising to rt. Reaction mass was diluted with water (30 mL) and extracted with EtOAc (2X50 mL). The combined organic layer was washed with brine (30 mL), dried over sodium sulfate and concentrated in vacuo. Purification by silica gel column chromatography (0 to 8% EtOAc in hexanes) afforded 5a as yellow solid (0.20 g, yield 45%). mp 173–175 °C.

\[ ^1H \text{NMR} (400 \text{ MHz, CDCl}_3) \delta 8.00 (d, J = 8.8 \text{ Hz}, 2H), 7.46 (dd, J = 8.0, 1.6 \text{ Hz}, 2H), 7.32 (t, J = 7.2 \text{ Hz}, 3H), 7.24–7.15 (m, 5H), 7.09–7.06 (m, 2H), 6.91 (d, J = 8.8 \text{ Hz}, 2H), 6.56 (d, J = 8.4 \text{ Hz}, 2H), 6.16 (s, 1H), 2.19 (s, 3H); \]

\[ ^{13}C \text{NMR} (100 \text{ MHz, CDCl}_3) \delta 167.47, 146.03, 141.03, 134.83, 133.78, 132.33, 132.30, 130.70, 130.46, 129.77, 129.46, 128.97, 128.63, 128.35, 128.25, 127.82, 126.41, 114.98, 114.64, 20.62; \]

HRMS (ESI) m/z: [M + H]^+ calcd for C_{29}H_{23}BrN_{3}O 508.1024; found 508.1009.

3-Phenyl-1-(phenylamino)-4-(p-tolyl)imidazo[5,1-b]quinazolin-9(4H)-one (6a).
CuI (6.0 mg, 0.03 mmol) was added to a degassed solution of compound 5a (200 mg, 0.34 mmol), K$_2$CO$_3$ (143 mg, 1.04 mmol), and (trans-N,N’-dimethylcyclohexane-1,2-diamine (10.0 mg, 0.07 mmol) in 1,4-dioxane (10 ml) and reaction mixture was stirred at 110°C for 16h. Reaction mass was cooled to rt, diluted with water (30 mL) and extracted with EtOAc (2X50 mL). The combined organic layer was washed with brine (30 mL), dried over sodium sulfate and concentrated in vacuo. Purification by silica gel column chromatography (0 to 5% EtOAc in hexanes) afforded 6a as yellow solid (95 mg, yield 65%). mp 227–230 °C. $^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.36 (d, $J = 7.2$ Hz, 1H), 7.78(dd, $J = 8.4$, 2.0 Hz, 2H), 7.50–7.43 (m, 4H), 7.15 (t, $J = 7.2$ Hz, 1H), 7.06–6.95 (m, 9H), 6.83 (d, $J = 8.4$ Hz, 1H), 2.27 (s, 3H); $^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 157.49, 142.70, 139.31, 139.07, 135.15, 134.02, 133.87, 131.83, 130.30, 130.28, 129.87, 129.38, 129.28, 129.21, 128.53, 127.36, 126.99, 125.86, 121.48, 120.94, 21.03; HRMS (ESI) m/z: [M + H]$^+$ calcd for C$_{29}$H$_{22}$N$_3$O 428.1763; found 428.1763.

**Abbreviations**

DCM, dichloromethane; TEA, triethylamine; 4-DMAP, 4-(dimethylamino)pyridine; MeOH, methanol; THF, tetrahydrofuran; EtOAc, ethyl acetate; HRMS, high-resolution mass spectrometry; mp, melting point.
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4a
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4a
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4b
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4b
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4c
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4c
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4d
$^3C$ NMR (100 MHz, methanol-$d_4$) spectrum of 4d
\(^1\)H NMR (400 MHz, methanol-\(d_4\)) spectrum of 4e
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4e
$^1\text{H} \text{NMR (} 400 \text{ MHz, methanol-d}_4 \text{)} \text{ spectrum of } 4\text{f}$
\(^{13}\)C NMR (100 MHz, methanol-\(d_4\)) spectrum of 4f
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4g
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4g
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4g
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4h
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4h
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4h
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4i
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4i
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4i
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4j
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4j
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4j
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4k
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4k

$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4k
MHz, methanol-\textit{d4}) spectrum of 4l
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4l
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4m
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4m
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4m
$^1$H NMR (400 MHz, methanol-d$_4$) spectrum of 4n
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4n
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4o
$^{13}$C NMR (100 MHz, methanol-\textit{d}_4) spectrum of 4o
$^1$H NMR (400 MHz, methanol-d$_4$) spectrum of 4p
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4p
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4q
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4q
\(^1\)H NMR (400 MHz, methanol-\(d_4\)) spectrum of 4r
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4r
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4s
$^{13}\text{C NMR (100 MHz, methanol-d$_4$) spectrum of 4s}$
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4t
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4t
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4u
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4u
\(^1\)H NMR (400 MHz, methanol-\(d_4\)) spectrum of \(4\nu\)
$^{13}$C NMR (100 MHz, methanol-\textit{d}_4) spectrum of \textit{4v}
$^{1}$H NMR (400 MHz, methanol-d$_4$) spectrum of 4w
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4w
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4x
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4y

AS-X-26-01
399.81
cd3ed
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4y
$^{19}$F NMR (376 MHz, methanol-\textit{d}$_4$) spectrum of 4y

$^1$H NMR (400 MHz)
\(^1\text{H NMR} (400 \text{ MHz, methanol-}d_4)\) spectrum of \(4z\)
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4z
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4z
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4aa
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4aa
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4aa
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ab
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ab
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4ab
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ac
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ac
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4ac
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ad
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ad
$^{19}\text{F NMR (376 MHz, methanol-$d_4$) spectrum of 4ad}$
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ae
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ae
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4af
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4af

[Chemical structure and spectrum image]
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ag
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ag
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ah
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ah
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ai

AS-X-32-H
399.81
cd590d

112
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ai
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4aj
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4aj
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ak
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ak
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4al
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4al
$^{19}\text{F NMR (376 MHz, methanol-}d_4\text{) spectrum of 4al}$
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4am
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4am
$^{19}$F NMR (376 MHz, methanol-$d_4$) spectrum of 4am
$^1$H NMR (400 MHz, methanol-d$_4$) spectrum of 4an
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4an
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ao
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ao
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4ap
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4ap
$^1$H NMR (400 MHz, methanol-$d_4$) spectrum of 4aq
$^{13}$C NMR (100 MHz, methanol-$d_4$) spectrum of 4aq
$^1$H NMR (400 MHz, CDCl3) spectrum of 5a
$^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of 5a
$^1$H NMR (400 MHz, CDCl3) spectrum of 6a
$^{13}$C NMR (100 MHz, CDCl$_3$) spectrum of 6a
Compound 4a

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0.500 H: 0.1000 N: 0.10
AS-X-07 74 (1.310)
1: TOF MS ES+

Minimum: -1.5
Maximum: 5.0 10.0 50.0
Mass Calc. Mass m/z PPM DBE i-FIT Norm Conf(k) Formula
326.1648 326.1657 -0.9 -2.8 14.5 644.3 n/a n/a C22 H20 N3

[+H]^+ : C22H20N3
Exact Mass: 326.1657

AS-X-07 74 (1.310)
326.1648
Compound 4b

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa  /  DBE: min = -1.5, max = 50.0
Element prediction: OT
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
48 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)

Elements Used:
C: 0-500  H: 0-1000  N: 0-10

KHM-III-58 70 (1.241)
1: TOF MS ES+

Minimum: 312.1489
Maximum: 312.1501

Mass  Calc. Mass mDa  PPM  DBE  I-FIT  Norm  Conform  Formula
312.1489  312.1501  -1.2  -1.8  14.5  542.0  n/a  n/a  C21 H18 N3

\[ \text{[M+H]^+}: C_{21}H_{18}N_3 \]
Exact Mass: 312.1501
**Compound 4c**

**Elemental Composition Report**

**Single Mass Analysis**
- Tolerance: 5.0 mDa / DBE: min = -1.5, max = 50.0
- Element prediction: Off
- Number of isotope peaks used for i-FIT = 3

**Monoisotopic Mass, Even Electron Ions**
- 54 formula(e) evaluated with 1 results within limits (all results up to 1000) for each mass
- Elements Used:
  - C: 0-500
  - H: 0-1000
  - N: 0-10

**AS-X-23 ESI**
- 1: TOF MS ES+

**[M+H]^+**: C_{23}H_{20}N_{3}

**Exact Mass**: 368.2127
Compound 4d

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
570 formulas evaluated with 5 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  O: 0-20
KHM-III-59 70 (1.241)
1: TOF MS ES+

Minimum:  Max. 5.0  10.0  50.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Norm  Conf(%)  Formula
342.1595  342.1606 -1.1  -3.2  14.5  618.2  0.194  82.40  C22 H20 N3 O
342.1586  2.9  8.8  15.5  619.8  1.761  17.19  C19 H20 N3 O
342.1553  2.2  12.3  9.5  623.3  3.754  3.75  C16 H24 N4
342.1638  -8.3  12.6  6.5  626.6  3.363  0.02  C11 H20 N5 O
342.1625  -3.0  -8.8  1.5  628.6  8.784  0.02  C10 H24 N5 O

[M+H]+: C22H20N3O
Exact Mass: 342.1606

[Diagram of molecular structure with molecular formula and mass spectrum graph]
### Compound 4e

**Elemental Composition Report**

**Single Mass Analysis**

- Tolerance: 5.0 mDa
- DBE: min = -1.5, max = 50.0
- Element prediction: Off
- Number of isotope peaks used for I-PIF = 3

**Monoisotopic Mass, Even Electron Ions**

169 formula(e) evaluated with 2 results within limits (all results up to 1000) for each mass

**Elements Used**

- C: 0.500
- H: 0.100
- N: 0.10
- Br: 0.8

**AS-X:11 75 (1.327)**

<table>
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<th>Mass</th>
<th>Calc. Mass</th>
<th>m/z</th>
<th>DBE</th>
<th>I-PIF</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
</tr>
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<tbody>
<tr>
<td>390.0598</td>
<td>390.0606</td>
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<td>14.5</td>
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**[M+H]+**: C21H17N3Br

**Exact Mass**: 390.0606
Compound 4f

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
257 formulas evaluated with 5 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  Cl: 0-8
AS-X-10 100 (1.772)

1: TOF MS ES+

2.42e5

Minimum: 1.5
Maximum: 10.0

Mass  Calr. Mass  m/z  PPM  DBE  i-FIT  Norm  Conf(%)  Formula
346.1100  346.1111  -3.2  14.5  241.7  0.001  99.88  C21 H17 N3 Cl
346.1120  -2.9  9.5  241.6  5.800  0.11  C20 H16 N3 Cl2
346.1062  3.8  13.9  6.5  252.2  10.359  0.00  C19 H16 N3 Cl2
346.1081  1.9  5.5  1.3  252.9  11.207  0.00  C18 H16 N3 Cl3
346.1093  0.7  2.6  19.5  259.2  17.523  0.00  C22 H12 N3

Exact Mass: 346.1111

[Mass] +: C21H17N3Cl

1. TOF MS ES+

3.12e6

AS-X-10

3.12e6

AS-X-10
Compound 4g

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-PIT = 3

Monoisotopic Mass, Even Electron Ions
360 formula(e) evaluated with 3 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  F: 0-10
AS X: 20-80 (1.421)

1: TOF MS ES+

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<th>Mass</th>
<th>Calc. Mass mDa</th>
<th>DPM</th>
<th>DBE</th>
<th>i-PIT</th>
<th>Norm</th>
<th>Conf(%)</th>
<th>Formula</th>
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<td>330.1397</td>
<td>330.1407</td>
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<td>-3.0</td>
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<tr>
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<td>13.99</td>
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<tr>
<td>330.1403</td>
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<td>-1.8</td>
<td>7.5</td>
<td>544.3</td>
<td>4.513</td>
<td>1.10</td>
<td>C11 H15 N9 P3</td>
</tr>
</tbody>
</table>

[M+H]+: C21H17N3F
Exact Mass: 330.1407
Compound 4h

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
300 formula(e) evaluated with 3 results within limits (all results up to 1000) for each mass

Elements Used:
C: 0-500 H: 0-1000 N: 0-10 F: 0-10

AS-X-16 70 (1.241)
1: TOF MS Es+

|M+H|: C_{21}H_{17}N_{3}F
Exact Mass: 330.1407
Compound 4i

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
360 formula(s) evaluated with 3 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  F: 0-10

$[\text{M+H}]^+$: C$_{21}$H$_{17}$N$_2$F
Exact Mass: 330.1407

\[ \text{Mass Calc.} \quad \text{Mass mol} \quad \text{mDa} \quad \text{DBE} \quad \text{i-FIT} \quad \text{Norm} \quad \text{Conf(%) Formula} \]

330.1397  330.1407  -0.6  -3.0  14.5  612.9  0.024  97.65  C$_{21}$H$_{17}$N$_2$F
330.1405  -0.6  -2.4  3.5  616.6  3.762  2.32  C$_{13}$H$_{18}$N$_3$F
330.1403  -0.6  -1.8  7.5  621.3  8.470  0.02  C$_{11}$H$_{15}$N$_5$F

AS-X-09 73 (1.293)
1: TOF MS ES+

3. Diode Array
Range: 2.66kA

1: TOF MS ES+
SPH
2.82e6

AS-X-09

1: TOF MS ES+
TIC
3.82e6

144
Compound 4j

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1179 formulas evaluated with 7 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0.500 H: 0.100 N: 0.10 F: 0.10 Br: 0.8

AS-X-17 Br (1.609)
1: TOF MS ESI+

[\text{M+H}]^+; \text{C}_{21}\text{H}_{16}\text{N}_3\text{FBr}

Exact Mass: 408.0512
Compound 4k

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
179 formula(s) evaluated with 2 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

AS-X-21 90 (1.593)
1: TOF MS ES+

Minimum: 1.5
Maximum: 5.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Norm  Conf(%)  Formula
404.0753  404.0762  -0.9  -2.2  14.5  558.4  0.000  100.00  C22 H19 N3 Br
404.0773  404.0782  -2.0  -0.9  -0.5  568.4  9.945  0.00  C10 H28 N7 Br2

 Exact Mass: 404.0762
Compound 41

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
179 formula(e) evaluated with 2 results within limits (up to 1000) for each mass
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  Br: 0-8

AS-X-24 84 (1.490)
1: TOF MS ES+

1.00e6

Minimum: 5.0  10.0  50.0
Maximum: 5.0  10.0  50.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Norm  Conf(%)  Formula
404.0755  404.0756  -0.7  -1.7  14.5  512.8  0.000  99.99  C22 H19 N3 Br
404.0773  -1.8  -4.5  -0.5  522.6  9.843  0.01  C10 H7 N7 Br2

[M+H]+: C22H19N3Br
Exact Mass: 404.0762
Compound 4m

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
431 formula(e) evaluated with 6 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  F: 0-10

AS-X-22 79 (1.404)

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<th>Calc. Mass</th>
<th>mDa</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
<th>Conf(k)</th>
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AS-X-22 79 (1.404)

[\text{M+H}]^+ : \text{C}_{22}\text{H}_{13}\text{N}_{3}\text{F}_3

Exact Mass: 380.1375

148
**Compound 4n**

**Elemental Composition Report**

**Single Mass Analysis**
- Tolerance = 5.0 mDa  
- DEE: min = -1.5, max = 50.0
- Element prediction: Off
- Number of isotope peaks used for i-FIT = 3

**Monoisotopic Mass, Even Electron Ions**
- 859 formulas evaluated with 7 results within limits (all results up to 1000) for each mass
- Elements Used:
  - C: 0-500
  - H: 0-1000
  - N: 0-10
  - O: 0-20

- [M+H]^+ \( \text{C}_{23}\text{H}_{20}\text{N}_{2}\text{O}_{2} \)
- Exact Mass: 370.1556

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<th>PPM</th>
<th>DEE</th>
<th>i-FIT</th>
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<td>0.01</td>
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<tr>
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<td>0.00</td>
<td>C8 H28 N8 011</td>
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**AS-X-14**

1: TOF MS ES+

**AS-X-14**

3: Diode Array
- Range: 2.877

**AS-X-14**

1: TOF MS ES+
- Range: 2.23e5

**AS-X-14**

1: TOF MS ES+
- Range: 3.15e6
Compound 4o

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa  /  DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
51 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500  H: 0-1000  N: 0-10
AS-X 1275 (1.328)
1. TOF MS ES+

\[
\text{[M+H]^+}: \ C_{22}H_{17}N_4
\]
Exact Mass: 337.1453
Compound 4p

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa  /  DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
632 formula(e) evaluated with 9 results within limits (all results up to 1000 for each mass)
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  O: 0-20
AS-X 1.37 (3.20)
1: TOF MS ES+

Minimum: 1.5
Maximum: 5.0  10.0  50.0
Mass Calcd. Mass eDa  DBE  i-FIT  Norm  Conf(%)  Formula
357.1348 357.1325 2.3 6.4 16.5 456.6 0.003 99.73  C17 H13 N10
357.1331 3.7 16.4 11.5 440.8 6.292 0.020  C14 H17 N6 O4
357.1352 -0.4 -1.1 15.5 444.3 7.768 0.040  C15 H17 N6 O2
357.1338 1.0 2.8 13.5 456.5 8.587 0.022  C20 H21 N6 O2
357.1370 -2.0 -4.2 2.5 467.3 10.699 0.000  C9 H21 N6 O2
357.1367 -4.0 -6.2 0.5 468.3 10.899 0.000  C9 H21 N6 O2
357.1357 -0.4 -1.1 15.5 440.8 6.292 0.020  C14 H17 N6 O4
357.1397 -4.4 -12.2 10.5 454.9 12.557 0.000  C13 H25 N11
357.1392 -4.4 -12.2 10.5 454.9 12.557 0.000  C13 H25 N11
357.1350 1.0 5.0 -1.5 454.9 12.557 0.000  C4 H21 N6 O11

(M+H): C23H17N2O2
Exact Mass: 357.1352
Compound 4q

[M+H]⁺: C_{23}H_{20}N_{5}

Exact Mass: 366.1719
Compound 4r

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element precision: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
176 formulas evaluated with 2 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 \( \text{H: 0-1000} \) \( \text{N: 0-10} \) \( \text{Br: 0-8} \)

\[
\begin{array}{cccccc}
\text{AS-X-25} & 404.0755 & 619.2154 & 809.1480 & 1044.2664 & 1597.7222 \\
\text{ES} & 1.19e+05 & 1.19e+05 & 1.19e+05 & 1.19e+05 & 1.19e+05 \\
\end{array}
\]

Minimum  1.5
Maximum  10.0  50.0

Mass  Calc. Mass  mDa  PPM  DBE  i-FIT  Norm  Conc.%  Formula
404.0755  404.0762  -0.7  -1.7  16.5  523.4  0.000  100.00  C22 H19 N3 Br
404.0773  -1.8  -4.3  -1.0  514.2  10.763  0.00  C10 H29 N7 Br2

\[
\begin{array}{cccccc}
\text{AS-X-25} & 404.0764 & 619.2154 & 809.1480 & 1214.2161 & 1597.7222 \\
\text{ES} & 1.19e+05 & 1.19e+05 & 1.19e+05 & 1.19e+05 & 1.19e+05 \\
\end{array}
\]

3: Diode Array
Range: 2.879

\[
\begin{array}{cccccc}
\text{AS-X-25} & 404.0764 & 619.2154 & 809.1480 & 1214.2161 & 1597.7222 \\
\text{ES} & 1.19e+05 & 1.19e+05 & 1.19e+05 & 1.19e+05 & 1.19e+05 \\
\end{array}
\]

[M+H]^+; C_{22}H_{19}BrN_3
Exact Mass: 404.0762
Compound 4s

Elemental Composition Report

Single Mass Analysis
Tolerance = 3.0 ppm
DBE: min = 1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for I-FlT = 3

Monosaccharide Mass, Even Electron ion
1856 results evaluated with 17 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20 Br: 0-8

[M+H]^+: C_{22}H_{19}N_{2}OBr
Exact Mass: 420.0712
Compound 4t

Elemental Composition Report

Single Mass Analysis
Tolerance = 1.0 ppm  /  DBE: min = 1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monotopic Mass, Elve Electroton time

Elemental formula evaluated with 10 results within limits (all results up to 1000) for each mass

Number of results: 10

Result:

\[ \text{[M+H]}^+ : \text{C}_{23}\text{H}_{19}\text{N}_3\text{OBr} \]

Exact Mass: 420.0712
**Compound 4u**

**Elemental Composition Report**

**Single Mass Analysis**
- Tolerance = 0.0105
- MIN = 0.5, max = 50.0
- Element prediction: Off
- Number of isotope peaks used for I/FIT: 9

**Monoisotropic Mass, Even Electron Loss**
- Results within limits (all results up to 1000) for each mass

**Elements Used**
- C: 50.0, H: 4.0, O: 10.0, N: 15.0, Br: 8.0

**AS-X-34 74 (1.319)**

[M+H]^+ : C_{22}H_{22}BrNO_2

Exact Mass: 434.0504

---

**AS-X-34 454**

1: TOF MS ES^+ 6.87e5
Compound 4v

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa  DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
252 formula(s) evaluated with 2 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  Br: 0-8
KHM-III-79 94 (1.061)
1: TOF MS ES+

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<th>Calc. Mass</th>
<th>Mea</th>
<th>PPM</th>
<th>DBE</th>
<th>i-FIT</th>
<th>Norm</th>
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<th>Formula</th>
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<td>-1.9</td>
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<td>99.82</td>
<td>C9 H16 N3 Br2</td>
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<tr>
<td>467.9722</td>
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<td>-0.5</td>
<td>410.2</td>
<td>6.341</td>
<td>0.18</td>
<td>C9 H25 N7 Br3</td>
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[M+H]+: C9H16N3Br2
Exact Mass: 467.9711
Compound 4w

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
292 formula(e) evaluated with 2 results within limits (all results up to 1000) for each mass

Elements Used:
C: 0.500  H: 0-1000  N: 0-10  Br: 0-8

AS-X 36 98 (1.739)
1: TOF MS ESI+

MINIMUM: -1.5
MAXIMUM: 5.0  10.0  50.0

Mass   Calc. Mass   mDa   FWM   DBE   i-FIT   Norm   Conf(%)   Formula
467.9703 467.9711  -0.8  -1.7  14.5  276.5  0.006  99.37  C21 H16 N3 Br2
447.9722  -1.9  -4.1  -0.5  281.6  5.068  0.63  CH25 N7 Br3

[1+H]+: C21H16N3Br
Exact Mass: 467.9711
Compound 4x

Elemental Composition Report

Single Mass Analysis
Tolerance = 0.0 mDa / OEE: min = -1.5, max = 5.0
Element prediction: CI
Number of isotopic peaks used for S/FIT = 3

Mass Spectrometric Analysis:
Selected mass spectra with 11 results within limits (all results up to 1000 m/z for each mass)

Elements Used:
C: 2.5% N: 16.0% Cl: 0.8% Br: 0.8%

AS-X-35 92 (1.628)

[M+H]^+: C_{28}H_{18}N_{4}ClBr
Exact Mass: 424.0216
Compound 4y

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for I-FFIT = 3

Monoisotopic Mass, Even Electron Ions
1179 formulas evaluated with 7 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0.950  H: 0.100  N: 0.10  Br: 0.8  F: 0.10

AS-X 02 82 (1.456)
1: TOF MS Es+ 1.08±0.06

100
285.1015  408.0502

Minimum: 1.5
Maximum: 5.0  10.0  50.0
Calc. Mass  mDa  PPm  DBE  I-FFIT  Mean  Conf (%): Formula
408.0502  408.0510 -1.9 -2.5 14.5  573.8  0.160  85.23 C21 H16 N2 Br F
409.0509 -0.6 -1.5 7.5  571.1  3.402  3.26 C19 H14 Br Br F3
409.0508 -2.9 -4.9 -9.5  562.4  9.767  0.01 C19 H14 Br Br F3
409.0504  4.0 9.6 -9.5  584.4  19.94  0.01 C22 H16 N2 Br3 F2
409.0505  0.7 1.7 11.5  594.0  22.49  0.01 C19 H14 Br Br F3
409.0507  0.5 1.2 22.5  593.0  21.136  0.00 C22 H16 Br3 F2

AS-X 26 82 (1.456)
1: TOF MS Es+ 1.08±0.06

100
408.0502

AS-X 26 100
411.0510

3: Diode Array
Range: 2.56

AS-X 26 100
1: TOF MS Es+

1: TOF MS Es+

[+H]$: C21H16N2BrF
Exact Mass: 408.0512
Compound 4z

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = 1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1784 formulas evaluated with 7 results within limits (all results up to 1000 for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8 F: 0-10

Minimum: 314
Maximum: 450

Mass Calcd. Mass sDa PPM DBE i-FIT Score Conf. (t) Formula
408.0499 408.051 2.1 0.3 145.6 472.5 0.162 85.94 C21 H16 N3 Br F
408.0510 408.051 2.7 0.3 145.6 472.5 0.162 85.94 C21 H16 N3 Br F
408.0509 408.051 2.7 0.3 145.6 472.5 0.162 85.94 C21 H16 N3 Br F
408.0502 408.051 2.7 0.3 145.6 472.5 0.162 85.94 C21 H16 N3 Br F
408.0497 408.051 2.7 0.3 145.6 472.5 0.162 85.94 C21 H16 N3 Br F

[+H]+: C21H16N3BrF
Exact Mass: 408.0512

3: Diode Array
Range: 0.568

1: TOF MS ES+
9.16e5
Compound 4aa

Elemental Composition Report

Single Mass Analysis
Tolerance = 0.0 mDa / DDE: min = 1.5, max = 50.0
Element prediction: Off
Number of isotopic peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ion
1295 formulae evaluated with 9 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0.500  H: 0.100  N: 0.10  Br: 0.8  F: 0.15

AS-X-29 91 (1.510)
1: TOF MS ES+

[M+H]⁺: C₂₁H₁₂N₂BrF₂
Exact Mass: 426.0417
Compound 4ab

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions (200 formula) evaluated within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  F: 0-10  Br: 0-8

[M+H]^+: C_{21}H_{14}N_{3}BrF_{2}
Exact Mass: 426.0417
Compound 4ac

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediciton: O
Number of isotope peaks used for I-FIT = 3
Monoisotopic Mass, Eanes Electron Ion
(1D mass spec) evaluated with 11 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500 H:0-100 N:0-10 F:0-10 Br:0-8

[M+H]+: C22H16N4F3Br
Exact Mass: 458.0480
Compound 4ad

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = 1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FT: 3

Monoisotopic Mass. Even Electron Ions
1528 formulae evaluated with 11 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 9-9.0 H: 0-100 N: 0-10 P: 0-10 Br: 0-9

AS-X-30 81 (1.438)
1: TOF MS ES+

[\text{M+H}^+]^*: \text{C}_{20}\text{H}_{10}\text{N}_{3}\text{F}_{3}\text{Br}

Exact Mass: 458.0480
Compound 4ac

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for >FIT = 3

Monoisotopic Mass, Even Electron loss
448 formula(s) evaluated with 6 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500  H: 0-1000  N: 0-10  S: 0-2  Br: 0-9

AS-X-28 0.3 (1.472)
1: TOF MS ES+

Mass  %Calc. Mass  mDa  ppm  DBE  >FIT  Norm  Conf(%)  Formula
394.0144  394.0104  -4.0  -10.1  8.6  491.7  555  55.15  C16 H13 N3 S Br
396.0170  -0.6  -11.6  13.5  481.9  0.421  43.98  C15 H15 N3 S Br
396.0134  2.8  7.1  18.6  485.8  0.750  0.87  C15 H15 N3 S Br
396.0147  1.7  6.3  3.5  491.5  10.472  0.00  C10 H26 N7 S Br2
396.0181  -1.7  -4.3  -1.5  493.1  12.027  0.00  C7 H24 N7 S Br2
396.0126  3.9  5.6  20.6  495.2  14.128  0.00  C15 H15 N3 S E2

[M+H]^+: C_{16}H_{13}N_{3}SBr
Exact Mass: 396.0170

166
**Compound 4af**

**Elemental Composition Report**

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<th>DE</th>
<th>i-FIT</th>
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</table>

**Monoisotopic Mass, Even Electron Ions**

209 formulae evaluated with 2 results within limits (all results (up to 1000) for each mass)

**Elements Used:**

- C: 0.500
- H: 0-1000
- N: 0-10
- Br: 0-8

**Exact Mass:** 440.0762
Compound 4ag

**Elemental Composition Report**

**Single Mass Analysis**
- Tolerance = 0.0 match
- DBE: min = 1.5, max = 50.0
- Element prediction: Off

**Number of Isotope peaks used for I-PI = 3**

**Monoisotopic Ions, Even Electron loss**
- 2610 formulas evaluated with 19 results within limits (all results up to 100(5) for each mass)

**Elements Used**
- C: 0-60, H: 0-100, N: 0-10, O: 0-10, Br: 0-10

**[M+H]+: C_{26}H_{20}N_2OBr**

**Exact Mass:** 470.0868
Compound 4ah

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
179 formula(e) evaluated with 2 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-000 H: 0-000 N: 0-10 Br: 0-8

[M+H]^+: C_{22}H_{19}N_{2}Br
Exact Mass: 404.0762

[Image of Mass Spectrogram]
Compound 4ai

Elemental Composition Report

Single Mass Analysis
Tolerance = 0.0025 / 0.1% mass = 16.6, mass = 50.0
Element prediction: Off
Number of complex peaks used for Off = 3

Monoisotopic Mass, Even Electron ion
sX formulae evaluated with 16 results active limits (all results up to 1000) for each mass
Elements Used:
C: 0.500  H: 0.600  N: 0.10  O: 0.20  Br: 0.0

Mass  DHE  DHE  [M+H]+  ConfId  Formula
420.2649  2.0  0.7  10.7  377.0  0.67  0.673  CHN0  0.03  0.03  0.03  0.03
420.2772  2.3  2.0  14.3  380.9  3.20  2.758  C20H12  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
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420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
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420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03
420.2775  4.1  5.4  7.6  102.7  2.96  2.956  C20H12N  0.03  0.03  0.03  0.03

[M+H]+: C20H12N5OBr
Exact Mass: 420.0712
**Compound 4aj**

**Elemental Composition Report**

**Single Mass Analysis**

- Tolerance: ±5.0 mDa
- DBE: min = -1.5, max = 50.0
- Element prediction: Off
- Number of isotope peaks used for i-FIT = 3

**Monoisotopic Mass, Even Electron Ions**

252 formula(e) evaluated with 2 results within limits (all results (up to 1000) for each mass)

**Elements Used:**
- C: 0-550
- H: 0-1000
- N: 0-10
- Br: 0-8

**KIHM III-75 104 (1.841)**

1: TOF MS ES+

- [M+H]+: C21H16N3Br2
- Exact Mass: 467.9711
**Compound 4ak**

**Elemental Composition Report**

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = 15, max = 50.0
Element prediction: C6H
Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions
666 formulae evaluated with 12 results within limits (all results up to 1000) for each mass

Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Cl: 0-8 Br: 0-8

**[M+H]^+**: C_{21}H_{16}N_{2}ClBr
Exact Mass: 424.0216
Compound 4al

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: C/H
Number of isotopic peaks used for i-PIT = 3

Monoisotopic Mass, Even Electron ions (1176 formula(e) evaluated with 7 results within limits (all results up to 1000) for each mass):
Elements Used:
C: 0-550  H: 0-1600  N: 0-10  Br: 0-8  F: 0-10
KHM-III-77 95 (1.679) 7.18e-005

Mass  Calc. Mass  mDa  PPM  DBE  i-PIT  Norm  Conf(%)  Formula
408.0497  408.0512  -1.5  3.7  145  516.2  0.115  89.16  C11 H16 N3 Br F
409.0510  -1.3  -3.2  2.5  518.6  2.655  8.59  C13 H17 N3 Br F
409.0508  -1.1  -2.7  1.5  519.9  3.795  2.25  C11 H14 N9 Br F3
409.0522  -2.3  -6.1  0.5  526.3  10.168  0.00  C9 H25 N7 Br2 F
409.0482  3.5  9.6  -0.5  526.4  10.325  0.00  C12 H26 N3 Br2 F2
409.0495  0.2  0.5  11.0  537.3  21.195  0.00  C15 H6 N5 F3
408.0497  0.0  0.0  22.5  537.4  21.300  0.00  C23 H5 N5 F3

[M+H]+: C23H16N3FBr
Exact Mass: 408.0512
Compound 4am

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = 1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron ions
M/Z formula (m/z) evaluated with 11 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-5000  N: 0-1000  Br: 0-10  F: 0-10

AS-X-33 105 (1.859)
1: TOF MS ES+

Minimum: 5.0 50.0
Maximum: 1.0 50.0

Mass  Calc. Mass  m/z  % PPM  DBE  I-FIT  Norm  Conf (%)
458.0473 458.0473 1.0 10.0 50.0

[M+H]^+: C_{22}H_{16}N_{3}F_{6}Br
Exact Mass: 458.0480
Compound 4an

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 ppm / DDC min = 1.5, max = 50.0
Element prediction: Off

Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron ions.
2020 formulae evaluated with 32 results within limits (all results up to 1000 for each mass)
Elements Used:
C: 0.32; H: 0.32; N: 0.10; Br: 0.00; O: 0.8

KOHMA 7.68 (c=0.6)
1: TOF MS ESI

175

[M-H][+]: C_{19}H_{19}N_{4}O_{2}Br

Exact Mass: 435.0457
Compound 4ao

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions
171 formula(e) evaluated with 3 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 Br: 0-8

[+H]: C_{20}H_{16}N_{2}Br
Exact Mass: 391.0558
Compound 4ap

Elemental Composition Report

Single Mass Analysis
Tolerance = 5.0 mDa  /  DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron ions
161 formula(e) evaluated with 3 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0.600  H: 0.450  N: 0.40  Br: 0.8

AS-X38 140 (2.475)
1: TOF MS ES+

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[3+H]^+: C_{18}H_{24}N_9Br
Exact Mass: 380.0511
Compound 4aq

Elemental Composition Report

Single Mass Analysis

Tolerance = 5.0 mDa / SBE, DIF = 1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for IFF = 3

Monoisotopic Mass, Exact Electron Ions

2021-04-16 17:23:28 15 results within limits (all results up to 1000) for each mass
Elements Used:
C-H-N-O

AS-X-37 T3 (1.293)

1: TOF MS ES+

5.87e+05

[M+H]^+: C_{20}H_{25}BrN_{3}O_{2}

Exact Mass: 429.0926
Compound 5a

Single Mass Analysis
Tolerance = 5.0 mDa / DBE: min = 1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions
2006 formula(ies) evaluated with 22 results within limits (all results up to 1000) for each mass
Elements Used:
C: 0.500 H: 0.100 N: 0.100 O: 0.200 Br: 0.00

KHM-IV-4232 (2.260)
1: TOF MS ESI+

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Exact Mass: 508.1024

3: Diode Array
Range: 4.075

1: TOF MS ESI+
2.11e6
Compound 6a

Single Mass Analysis
Tolerance = 5.0 mDa / DEE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for I-FIT = 3

Monoisotopic Mass, Even Electron Ions
843 formula(e) evaluated with 7 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 0-500 H: 0-1000 N: 0-10 O: 0-20

WM: 51.62 117.0371 (0.071)
1: TOF MS ES+

Minimum: 2.00 10.00 50.00
Mass Calc. Mass mDa FPM DBS I-FIT Norm Cost(%) Formula
428.1763 428.1783 0.0 0.0 20.5 702.1 0.107 89.88 C29 H22 N3 O
428.1795 4.0 0.3 10.5 702.3 2.311 9.82 C24 H12 N5 O3
428.1723 -0.2 -7.5 12.5 707.1 7.048 0.99 C18 H12 N5 O4
428.1791 -1.8 -4.2 7.5 707.3 3.053 0.99 C17 H12 N5 O5
428.1768 -0.5 -1.3 2.5 708.4 9.962 0.02 C16 H10 N5 O5
428.1741 2.2 5.1 3.5 710.2 10.424 0.00 C12 H26 N7 O10
428.1728 3.5 6.2 -1.5 711.5 11.446 0.00 C11 H30 N7 O14

[M+H]+: C29H22N3O
Exact Mass: 428.1763

[Image of a molecule with a structure and mass spectrum]